

ABSTRACT OF THE DISCLOSURE

[00202] This present invention is directed towards the identification or design, preparation, and use of suitable transition metal complexes for use as catalysts. The transition metal complexes may comprise heterodonor ligands. The present invention is also directed toward a method of determining the suitability of a transition metal complex for use in a catalytic reaction, such as, but not limited to, atom transfer radical polymerization (“ATRP”), atom transfer radical addition (“ATRA”), atom transfer radical cyclization (“ATRC”), and other catalytic redox reactions. The method assists in the approximate determination of the fundamental properties of the transition metal complex in a reaction media, such as, but not limited to, solubility, redox potential, stability towards acidic, basic, or ionic species, conditional radically transferable atom phyllicity, and propensity toward disproportionation and therefore, the suitability of the complex to be used as a catalyst in the reaction media. The method provides a basis for prediction and evaluation of the properties of a transition metal complex for a particular selective catalytic reaction in a broad range of reaction environments. An understanding of the principles of the disclosed method allows a transition metal complex to be tuned to specific reaction medium by selecting a transition metal complex and ligand combination having the desired qualities.